

Volume 482  
December 31, 1986

## COMPUTER SIMULATION OF CHEMICAL AND BIOMOLECULAR SYSTEMS<sup>a</sup>

*Editors*

DAVID L. BEVERIDGE and WILLIAM L. JORGENSEN

---

### CONTENTS

---

Preface. By DAVID L. BEVERIDGE and WILLIAM L. JORGENSEN.....	ix
--	----

#### Part I. Procedures and Methodology

Free Energy Simulations. By M. MEZEI and D. L. BEVERIDGE .....	1
Computer Simulations of Macromolecular Dynamics: Models for Vibrational Spectroscopy and X-Ray Refinement. By RONALD M. LEVY .....	24
Nuclear Magnetic Resonance Relaxation and the Dynamics of Proteins and Membranes: Theory and Experiment. By ATTILA SZABO .....	44
Molecular Dynamics Simulation Study of Polypeptide Conformational Equilibria: A Progress Report. By AMIL ANDERSON, MIKE CARSON, and JAN HERMANS .....	51
Conformational Energy Calculations on Polypeptides and Proteins: Use of a Statistical Mechanical Procedure for Evaluating Structure and Properties. By HAROLD A. SCHERAGA and GREGORY H. PAINE.....	60
Computer Simulation of DNA Supercoiling. By WILMA K. OLSON and JANET CICARIELLO .....	69
Calculation of Atomic Charges in Large Molecules. By S. SHANKAR, W. J. MORTIER, and S. K. GHOSH .....	82
A Vectorized Near-Neighbors Algorithm of Order N for Molecular Dynamics Simulations. By S. G. LAMBRAKOS, J. P. BORIS, I. CHANDRASEKHAR, and B. GABER.....	85
A Comment on Hamiltonian Parameterization in Kirkwood Free Energy Calculations. By ALBERT J. CROSS .....	89

#### Part II. Aqueous Solutions

Dynamics of Coordinated Water: A Comparison of Experiment and Simulation Results. By P. A. MADDEN and R. W. IMPEY .....	91
Hydrophobic and Ionic Hydration Phenomena. By PETER J. ROSSKY .....	115

<sup>a</sup>This volume is the result of a conference entitled Computer Simulation of Chemical and Biomolecular Systems, which was held by the New York Academy of Sciences on October 2-4, 1985 in New York City.

Neutron Diffraction Studies of Aqueous Solutions of Molecules of Biological Importance: An Approach to Liquid-State Structural Chemistry. <i>By</i> J. L. FINNEY and J. TURNER .....	127
The Born Model of Ion Solvation Revisited. <i>By</i> ALEXANDER A. RASHIN and BARRY HONIG.....	143

### Part III. Crystal Hydrates

The Structure, Energy, Entropy, and Dynamics of Peptide Crystals. <i>By</i> D. H. KITSON, F. AVBELJ, D. S. EGGLESTON, and A. T. HAGLER .....	145
Progress in the Water Structure of the Protein Crambin by X-Ray Diffraction at 140 K. <i>By</i> MARTHA M. TEETER and HÅKON HOPE.....	163
Hydration of Nucleic Acid Crystals. <i>By</i> HELEN M. BERMAN .....	166
Monte Carlo Studies of Water in Crystal Hydrates. <i>By</i> JULIA M. GOODFELLOW, P. LYNNE HOWELL, and FRANÇOISE VOVELLE .....	179
Computer Simulation of Nucleotide Crystal Hydrates and Solutions. <i>By</i> P. LYNNE HOWELL and JULIA M. GOODFELLOW .....	195

### Part IV. Reactions and Interactions

Computer Simulations of Organic Reactions in Solution. <i>By</i> WILLIAM L. JORGENSEN, JAYARAMAN CHANDRASEKHAR, J. KATHLEEN BUCKNER, and JEFFRY D. MADURA.....	198
Ionic Association in Water: From Atoms to Enzymes. <i>By</i> J. ANDREW MCCAMMON, OMAR A. KARIM, TERRY P. LYBRAND, and CHUNG F. WONG .....	210
Dynamic Simulations of Oxygen Binding to Myoglobin. <i>By</i> DAVID A. CASE and J. ANDREW MCCAMMON.....	222
Modeling Complex Molecular Interactions Involving Proteins and DNA. <i>By</i> PETER A. KOLLMAN, SCOTT WEINER, GEORGE SEIBEL, TERRY LYBRAND, U. CHANDRA SINGH, JAMES CALDWELL, and SHASHIDHAR N. RAO.....	234
Salt Effects on Enzyme-Substrate Interactions by Monte Carlo Simulation. <i>By</i> R. J. BACQUET and J. A. MCCAMMON .....	245
Energy Minimization Calculations on the Alkali Metal Cation Complexes of Valinomycin. <i>By</i> JOSEPH N. KUSHICK and REMO A. MASUT .....	248
A Molecular Mechanics Study (AMBER) of the Displacement of Thyroxine from the Binding Pocket of Prealbumin by PCBs and PCB Analogues. <i>By</i> T. DARDEN, J. MCKINNEY, A. MAYNARD, S. OATLEY, and L. PEDERSEN ...	249
Theoretical Models of Spermine/DNA Interactions. <i>By</i> BURT G. FEUERSTEIN, NAGARAJAN PATTABIRAMAN, and LAURENCE J. MARTON .....	251

### Part V. Biomacromolecules

Molecular Dynamics: Applications to Proteins. <i>By</i> MARTIN KARPLUS .....	255
A Lysozyme Molecular Dynamics Simulation. <i>By</i> CAROL B. POST, MARTIN KARPLUS, and CHRISTOPHER DOBSON .....	267
Simulations of Proteins in Water. <i>By</i> H. J. C. BERENDSEN, W. F. VAN GUNSTEREN, H. R. J. ZWINDERMAN, and R. G. GEURTSSEN .....	269

A Molecular Dynamics Computer Simulation of an Eight-Base-Pair DNA Fragment in Aqueous Solution: Comparison with Experimental Two-Dimensional NMR Data. <i>By</i> W. F. VAN GUNSTEREN, H. J. C. BERENDSEN, R. G. GEURTSSEN, and H. R. J. ZWINDERMAN .....	287
Tryptophan Structure and Dynamics Using GROMOS. <i>By</i> RICHARD A. ENGH, LIN X. CHEN, and GRAHAM R. FLEMING .....	304
Index of Contributors .....	307

**Financial assistance was received from:**

- Burroughs Wellcome Co.
- Cemcomco
- E.I. du Pont de Nemours & Company—Biomedical Products Department
- ELXSI
- Gould Electronics—Computer Systems Division
- Hoffmann-LaRoche, Inc.
- Office of Naval Research, Department of the Navy (Grant N00014-85-G-0214)
- Rhône-Poulenc Inc.
- Smith Kline & French Laboratories
- Stuart Pharmaceuticals/Division of ICI Americas

The New York Academy of Sciences believes it has a responsibility to provide an open forum for discussion of scientific questions. The positions taken by the participants in the reported conferences are their own and not necessarily those of the Academy. The Academy has no intent to influence legislation by providing such forums.